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                 "Ask CAS" for self-help around the clock
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                alerts (SDIs) affected
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NEWS
                COMPUAB reloaded; updating to resume; current-awareness
                alerts (SDIs) affected
NEWS
    11 DEC 17
                SOLIDSTATE reloaded; updating to resume; current-awareness
                alerts (SDIs) affected
     12 DEC 17
                CERAB reloaded; updating to resume; current-awareness
                alerts (SDIs) affected
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    13 DEC 17
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     14 DEC 30
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    15 DEC 30
                CAPLUS - PATENT COVERAGE EXPANDED
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                February 2005
NEWS 17 FEB 25 CA/CAPLUS - Russian Agency for Patents and Trademarks
                 (ROSPATENT) added to list of core patent offices covered
NEWS 18 FEB 10
                STN Patent Forums to be held in March 2005
NEWS 19 FEB 16 STN User Update to be held in conjunction with the 229th ACS
                National Meeting on March 13, 2005
NEWS 20 FEB 28 PATDPAFULL - New display fields provide for legal status
                data from INPADOC
NEWS 21 FEB 28 BABS - Current-awareness alerts (SDIs) available
NEWS 22 FEB 28 MEDLINE/LMEDLINE reloaded
NEWS 23 MAR 02
                GBFULL: New full-text patent database on STN
NEWS 24 MAR 03 REGISTRY/ZREGISTRY - Sequence annotations enhanced
NEWS EXPRESS JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT
              MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
              AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005
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STRUCTURE FILE UPDATES: 2 MAR 2005 HIGHEST RN 841200-41-7 DICTIONARY FILE UPDATES: 2 MAR 2005 HIGHEST RN 841200-41-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

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Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=>

Uploading C:\Program Files\Stnexp\Queries\10784916b.str

chain nodes :

1 2 3 4 5 6 7 8 9 10 11 19 20 21 22 23 30 31 33 34 ring nodes:
13 14 15 16 17 18 24 25 26 27 28 29 chain bonds:
1-2 1-33 1-34 2-3 2-22 2-23 3-4 3-21 4-5 4-20 5-6 6-7 6-19 7-8 7-11 8-9 9-10 10-30 10-31 10-25 18-19 ring bonds:
13-14 13-18 14-15 15-16 16-17 17-18 24-25 24-29 25-26 26-27 27-28 28-29 exact/norm bonds:
4-5 4-20 5-6 7-11 8-9 9-10 10-30 10-31 10-25 exact bonds:
1-2 2-3 2-22 2-23 3-4 3-21 6-7 6-19 7-8 18-19 normalized bonds:
1-33 1-34 13-14 13-18 14-15 15-16 16-17 17-18 24-25 24-29 25-26 26-27 27-28 28-29

Hydrogen count:

11:= exact 1 34:= exact 1

Connectivity:

9:3 M minimum RC ring/chain

Match level:

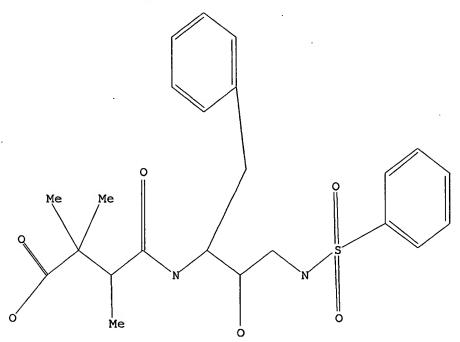
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS

10:CLASS 11:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS

20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:CLASS 31:CLASS 33:CLASS 34:CLASS

## L1 STRUCTURE UPLOADED

=> d L1 HAS NO ANSWERS L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s L1

SAMPLE SEARCH INITIATED 14:20:43 FILE 'REGISTRY' 46 TO ITERATE SAMPLE SCREEN SEARCH COMPLETED -

**46 ITERATIONS** 100.0% PROCESSED

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

> BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS:

514 TO 1326

PROJECTED ANSWERS:

0 TO

L2

L3

0 SEA SSS SAM L1

5 SEA SSS FUL L1

=> s L1 full

FULL SEARCH INITIATED 14:20:47 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED -877 TO ITERATE

100.0% PROCESSED 877 ITERATIONS 5 ANSWERS

0 ANSWERS

SEARCH TIME: 00.00.01

=> fil caplus COST IN U.S. DOLLARS

SINCE FILE

TOTAL

FULL ESTIMATED COST

ENTRY SESSION 161.33 161.54

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FILE COVERS 1907 - 3 Mar 2005 VOL 142 ISS 10 FILE LAST UPDATED: 2 Mar 2005 (20050302/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s L3

L4

3 L3

=> d L4 ibib abs hitstr 1-3

ANSWER 1 OF 3 CAPLUS

ACCESSION NUMBER:

DOCUMENT NUMBER:

TITLE:

AUTHOR(S):

On STN

124:193129

Determination of protein binding by in vitro charcoal adsorption
Yuan, Jinhua; Yang, Dai Chang; Birkmeier, Jill;

ASSIMBLE

ASSIMBLE

Stolzenbach, James

CORPORATE SOURCE: Pharmacokinetics, Bioanalytical and Radiochemistry

Function, G. D. Searle Research and Development, Skokie, IL, 60077, USA

SOURCE:

Journal of Pharmacokinetics and Biopharmaceutics

(1995), 23(1), 41-55 SODEN: JPBPBJ; ISSN: 0090-466X

PUBLISHER: DOCUMENT TYPE:

IT

RŃ

ĆN

Plenum Journal English

LANGUAGE:

Certain compds. such as SC-52151 have extensive nonspecific adsorption to the ultrafiltration devices or to dialysis membranes and therefore can not be measured by the conventional ultrafiltration or equilibrium dialysis methods. A new method based on charcoal adsorption was developed to overcome this difficulty. Unlike many conventional methods, which are based on the separation of free drug from bound drug under equilibrium conditions,

the new method is operated under nonequil. conditions and involves measuring the time course of decline of the percentage of bound drug remaining in plasma while the free drug is being removed by charcoal adsorption. Theor. aspects of the method and the data processing procedure are presented. SC-98A, a compound with minimal nonspecific adsorption to the ultrafiltration membrane, was used to demonstrate the applicability of this method against the ultrafiltration method. Using this method, the protein binding of SC-52151 in human plasma at 1.0 μg/mL was determined to be in the range of 91.4-97.7% at room temperature 157445-98-2, SC 98A

RL: BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses) (protein binding determination by in vitro charcoal adsorption) 157445-98-2 CAPLUS

Butanoic\_acid 4-[[(15,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)ami nol=1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Ph HN CO2H Me

ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1995:964989 CAPLUS

DOCUMENT NUMBER:

124:176937

TITLE:

N-[(Succinoylamino)hydroxypropyl]sulfonamides useful

as retroviral protease inhibitors

INVENTOR(S):

Vazquez, Michael L.; Mueller, Richard A.; Talley, John

J.; Getman, Daniel; Decrescenzo, Gary A.; Freskos,

Jøhn N.

PATENT ASSIGNEE(S):

SOURCE:

G. D. Searle and Co., USA

U.S., 32 pp\_\_cont.-in-part of U.S. Ser. No. 935,490,

abandoned CODEN: USXXAM

DOCUMENT TYPE: LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
;	US 5463104	A	19951031	US 1993-110912	19930824
	AT 154800	E	19970715	AT 1993-920213	19930824
'n	ES 2103488	Т3	19970916	ES 1993-920213	19930824
h	US 5714605	Α	19980203	US 1995-541350	19951010
1440	US 5760076	A	19980602	US 1995-541747	19951010
part	US 6022994	Α	20000208	US 1998-41016	19980312
<i>y</i> .	US 6313345	B1	20011106	US 1999-419816	19991018
1	US 2002137942	A1	20020926	US 2001-884462	20010620
;	US 6469207	B2	20021022		
{	US 2003220508	A1	20031127	US 2002-237184	20020909
j	US 6727282	B2	20040427		
BULLO BLA	US 2005004043	A1	20050106	US 2004-784916	20040224
PRIC	RITY APPLN. INFO.:			US 1992-935490	B2 19920825
74				US 1993-110912	A3 19930824
				US 1995-541350	A1 19951010
				US 1995-541747	A1 19951010
				US 1998-41016	A1 19980312
				US 1999-419816	Al 19991018
				US 2001-884462	A1 20010620
			•	US 2002-237184	A1 20020909

OTHER SOURCE(S): MARPAT 124:176937 GI

AΒ Succinoylamino hydroxyethylamino sulfonamide compds. I or a pharmaceutically acceptable salt or ester thereof, wherein p represents 0,

1 or 2; n represents either 0 or 1; X' represents N(R34) or O; or R33X' represents cycloalkyl or aryl radicals; Y and Y' each independently represent O or S; R1, R30, R31 and R32 each independently represent hydrogen, OH, (CH2)C(O)CH3, CH2SO2NH2, CO2CH3, CONHCH3, CON(CH3)2, CH2C(O)NHCH3, CH2C(O)N(CH3)2, CONH2, C(CH3)2(SH), C(CH3)2(SCH3), C(CH3)2[S(O)CH3], C(CH3)2[S(O)2CH3], alkyl, haloalkyl, alkenyl, alkynyl, aralkyl or cycloalkyl radicals, or the side chain of the amino acid asparagine, S-Me cysteine or the corresponding sulfoxide or sulfone derivs. thereof, leucine, isoleucine, allo-isoleucine, tert-leucine, phenylalanine, ornithine, alanine, norleucine, glutamine, valine, threonine, serine, o-alkyl serine, aspartic acid,  $\beta$ -cyanoalanine or allothreonine; or R30 and R32 together with the carbon atoms to which they are attached form a cycloalkyl radical; R2 = e.g., alkyl, aryl, cycloalkyl; R3, R33, R34 = e.g., H, alkyl, haloalkyl; R4 = e.g., alkyl, haloalkyl, alkenyl; R6 = H, alkyl; are effective as retroviral protease inhibitors, and in particular as inhibitors of HIV protease. Thus, e.g., butanediamide II was prepared by coupling of benzyl (R)-2,2,3trimethylsuccinate (preparation given) with 2(R)-hydroxy-3-[(3methylbutyl)(phenylsulfonyl)amino]-1(S)-(phenylmethyl)propylamine (preparation given) followed by benzyl ester hydrogenolysis and amidation, and exhibited IC50 = 2 nM for inhibition of HIV protease.

IT 157445-98-2P 157446-00-9P 157446-03-2P 157446-09-8P 157474-44-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(N-[(succinoylamino)hydroxypropyl]sulfonamides useful as retroviral protease)inhibitors)

RN/ 157445-98-2/ CAPLUS

CN Butanoic acid, 4-[[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)ami no]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 157446-00-9 CAPLUS

CN Butanoic acid, 4-[[2-hydroxy-3-[(2-methylpropyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, [1S-[1R\*(S\*),2S\*]]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

157446-03-2 CAPLUS RN

Butanoic acid, 4-[[2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](2-CN methylpropyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, [1S-[1R\*(S\*),2S\*]]-(9CI)(ÇA INDEX NAME)

RN .157446-09-8 CAPLUS

yer perby Butanoic acid, 4-[[3-[[(4-fluorophenyl)sulfonyl](3-methylbutyl)amino]-2-CN hydroxy-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, [1S-[1R\*(S\*),2S\*]]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 157474-44-7 CAPLUS

Butanoic acid, 4-[[2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](3-CN methylbutyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, [1S-[1R\*(S\*),2S\*]]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:579258 CAPLUS

DOCUMENT NUMBER:

121:179258

TITLE:

N-(alkanoylamino-2-hydroxypropyl)sulfonamides useful

as HIV protease inhibitors

INVENTOR(S):

Vazquez, Michael L.; Mueller, Richard A.; Talley, John

J.; Getman, Daniel; Decrescenzo, Gary A.; Freskos,

John N.

PATENT ASSIGNEE(S):

G.D. Searle and Co., USA; Monsanto Co.

SOURCE:

PCT Int. Appl., 103 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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	PATENT NO.			KIND DATE			\	APPLICATION NO.					DATE					
	WO 9404491			<b>A</b> 1	19940303				WO 1993-US7815				19930825					
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	ΕP	6568	-	•	-	A1 19950614			•		• ,	•		•				
		6568																
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		2103										1993-						
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	ΑU	9350	819			A1		1994	0315									
	RU	2130	016			C1		1999	0510		RU	1995-	1068	23		1	9930	825
	NO	9500	670			Α		1995	0222			1995-					9950	222
	FI	9500	841			Α		1995	0223		FI	1995-	841			1	9950	223
PRIO	RIT	Y APP	LN.	INFO	. :						US	1992-	9354	90		A2 1	9920	825
											WO	1993-	บร78	15	,	W 1	9930	825
OTHER SOURCE(S).				MAD	ΡΔΨ	121.	1792	5.8										

OTHER SOURCE(S):

MARPAT 121:179258

GΙ

The title compds. R33(R34)X1C(:Y1)(CH2)tC(R31)(R32)C(R30)(R1)C(:Y)N(R6)C(R2)HC(OH)HCH2N(R3)S(O)xR4 [R1 = H, CH2SO2NH2, CO2Me, CONHMe, CONMe2, etc.; R2 = alkyl, aryl, cycloalkyl, (un)substituted cycloalkylalkyl and arylalkyl; R3 = H, alkyl, haloalkyl, alkenyl, alkynyl, hydroxyalkyl, alkoxyalkyl, cycloalkyl, etc.; R4 = alkyl, haloalkyl alkenyl, alkynyl, hydroxyalkyl, alkoxyalkyl, cycloalkyl etc.; R6 = H, alkyl; R30-R32 = R1; R1R30R31 = cycloalkyl; R1R30R32C = cycloalkyl; R33, R34 = H, R3; R33R34X1 = cycloalkyl, aryl, heterocyclyl, etc.; X1 = O, N, CR17; R17 = H, alkyl; Y, Y1 = O, S, NR15; R15 = H, R3; t = 0, 1; x = 0-2], useful as HIV protease inhibitors for the treatment of AIDS, are prepared Thus, sulfonamide I was prepared and demonstrated IC50 against HIV protease of 1 nmol.

IT · 157446-09-8 157474-44-7

RL: RCT (Reactant); RACT (Reactant or reagent)
 (HIV protease inhibitor)

RN 157446-09-8 CAPLUS

CN Butanoic acid, 4-[[3-[[(4-fluorophenyl)sulfonyl](3-methylbutyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-,
[1S-[1R\*(S\*),2S\*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 157474-44-7 CAPLUS

CN Butanoic acid, 4-[[2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](3-methylbutyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, [1S-[1R\*(S\*),2S\*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

## IT 157445-98-2P 157446-00-9P 157446-03-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of, as HIV protease inhibitor)

RN 157445-98-2 CAPLUS

CN Butanoic acid, 4-[[(1S,2R)-2-hydroxy-3-[(3-methylbutyl)(phenylsulfonyl)ami no]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 157446-00-9 CAPLUS

CN Butanoic acid, 4-[[2-hydroxy-3-[(2-methylpropyl)(phenylsulfonyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-, [1S-[1R\*(S\*),2S\*]]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 157446-03-2 CAPLUS

CN Butanoic acid, 4-[[2-hydroxy-3-[[(4-methoxyphenyl)sulfonyl](2-methylpropyl)amino]-1-(phenylmethyl)propyl]amino]-2,2,3-trimethyl-4-oxo-,
[1S-[1R\*(S\*),2S\*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

=> FIL STNGUIDE COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 17.07 178.61 SINCE FILE DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) TOTAL ENTRY SESSION CA SUBSCRIBER PRICE -2.19-2.19

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FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Feb 25, 2005 (20050225/UP).

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FULL ESTIMATED COST	ENTRY 0.24	SESSION 178.85		
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CA SUBSCRIBER PRICE	0.00	-2.19		

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